Simulation of Turbulent Premixed Hydrogen Combustion

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SIAM Conference on Computational Science and Engineering
Miami, FL
March 2-6, 2009

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Lean Premixed Turbulent Combustion

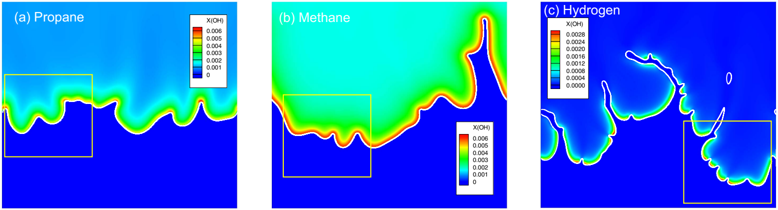
Rod-stabilized V-flame

4-jet Low-swirl burner (LSB)

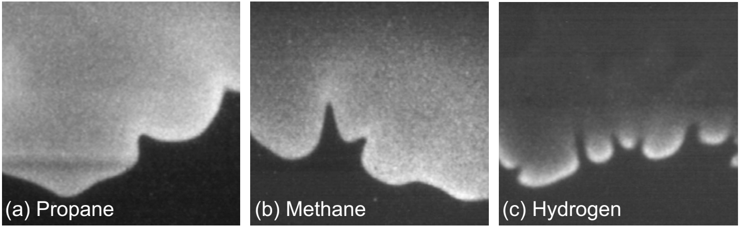
Slot burner

- Potential for efficient, low-emission power systems
- Design issues because of flame instabilities
- Focus on behavior of lean premixed hydrogen combustion

Fuel dependence of flame structure



OH Mole fraction



OH PLIF

Compressible Navier Stokes

Gas phase combustion – mixture model for diffusion

$$
\begin{aligned}
\textbf{Mass} \quad & \rho_t + \nabla \cdot \rho U = 0 \\
\textbf{Momentum} \quad & (\rho U)_t + \nabla \cdot (\rho U U + p) = \rho \vec{g} + \nabla \cdot \tau \\
\textbf{Energy} \quad & (\rho E)_t + \nabla \cdot (\rho U E + pU) = \nabla \cdot \kappa \nabla T + \nabla \cdot \tau U \\
& \qquad + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m) \\
\textbf{Species} \quad & (\rho Y_m)_t + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m
\end{aligned}
$$

Augmented with

- Thermodynamics
- Reaction kinetics
- Transport coefficients

Need to preserve chemical and transport fidelity

Relevant Scales

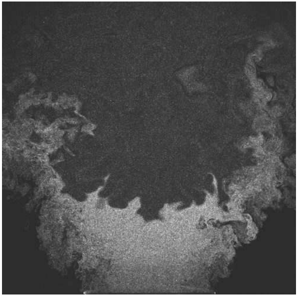
Spatial Scales

- Domain: $\approx$ 10 cm
- Flame thickness: $\delta_T \approx 1$ mm
- Integral scale: $\ell_t \approx 2 - 6$ mm

Temporal Scales

- Flame speed $O(10^2)$ cm/s
- Mean Flow: $O(10^3)$ cm/s
- Acoustic Speed: $O(10^5)$ cm/s

Fast chemical time scales but energy release coupling chemistry to fluid is on slower time scales



Mie Scattering Image

Low swirl burner simulation

Simulation requirements

- No explicit model for turbulence, or turbulence/chemistry interactions
- Detailed chemistry based on fundamental reactions, detailed diffusion
- Simulate on time scales associated with the fluid velocity

Direct integration of compressible Navier Stokes too demanding

Exploit structure of the problem

- Mathematical model
- Approximation / discretization
- Solvers and software

Mathematical formulation

Exploit natural separation of scales between fluid motion and acoustic wave propagation

Low Mach number model, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

Start with the compressible Navier-Stokes equations for multicomponent reacting flow, and expand in the Mach number, $M = U/c$.

Asymptotic analysis shows that:

$$p(\vec{x}, t) = p_0(t) + \pi(\vec{x}, t) \quad \text{where} \quad \pi/p_0 \sim \mathcal{O}(M^2)$$

- p_0 does not affect local dynamics, π does not affect thermodynamics
- For open containers p_0 is constant
- Pressure field is instantaneously equilibrated – removed acoustic wave propagation

Low Mach number equations

$$\textbf{Momentum}\quad \rho\frac{DU}{Dt} = -\nabla\pi + \nabla\cdot\left[\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot U\right)\right]$$

$$\textbf{Species}\quad \frac{\partial(\rho Y_m)}{\partial t} + \nabla\cdot(\rho U Y_m) = \nabla\cdot(\rho D_m \nabla Y_m) + \dot{\omega}_m$$

$$\textbf{Mass}\quad \frac{\partial\rho}{\partial t} + \nabla\cdot(\rho U) = 0$$

$$\textbf{Energy}\quad \frac{\partial\rho h}{\partial t} + \nabla\cdot\left(\rho h\vec{U}\right) = \nabla\cdot(\lambda\nabla T) + \sum_m \nabla\cdot(\rho h_m D_m \nabla Y_m)$$

Equation of state $p_0 = \rho\mathcal{R}T\sum_m \frac{Y_m}{W_m}$

System contains four evolution equations for U, Y_m, ρ, h, with a constraint given by the EOS.

Low Mach number system can be advanced at fluid time scale instead of acoustic time scale but . . .

We need effective integration techniques for this more complex formulation

Constraint for reacting flows

Low Mach number system is a system of PDE's evolving subject to a constraint; differential algebraic equation (DAE) with index 3

Differentiate constraint to reduce index

$$\nabla \cdot U = \frac{1}{\rho c_p T}\left(\nabla \cdot (\lambda \nabla T) + \sum_m \rho D_m \nabla Y_m \cdot \nabla h_m\right) + \frac{1}{\rho}\sum_m \frac{W}{W_m}\nabla(D_m \rho \nabla Y_m) + \frac{1}{\rho}\sum_m \left(\frac{W}{W_m} - \frac{h_m(T)}{c_p T}\right)\dot{\omega}_m$$

Generalized projection method framework

- Finite amplitude density variation
- Inhomogeneous constraint
- Requires solution of variable coefficient, self-adjoint elliptic PDE

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Low Mach number numerics

Fractional step scheme

- Advance velocity and thermodynamic variables
  - Advection
  - Diffusion
  - Stiff reactions
- Project solution back onto constraint – variable coefficient elliptic PDE, multigrid

Stiff kinetics relative to fluid dynamical time scales

$$\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$$

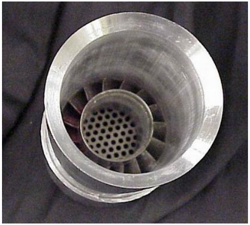
$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$$

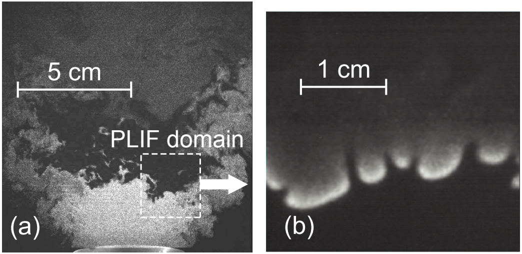
Operator split approach

- Chemistry $\Rightarrow \Delta t/2$
- Advection – Diffusion $\Rightarrow \Delta t$
- Chemistry $\Rightarrow \Delta t/2$

Coupled to block structured AMR

Hydrogen combustion

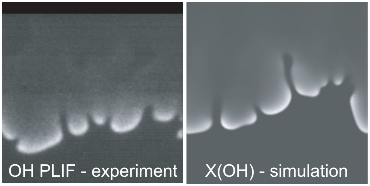


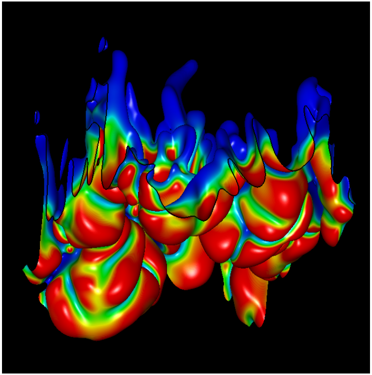


- OH PLIF shows gaps in the flame
- How do these flames burn?
- Are existing engineering models applicable?
- Can standard flame analysis techniques be used to analyze structure?

Hydrogen flame in 3D

3D control simulation of detailed hydrogen flame at laboratory scales ($3 \times 3 \times 9$ cm domain, $\Delta x_f = 58\mu$m)

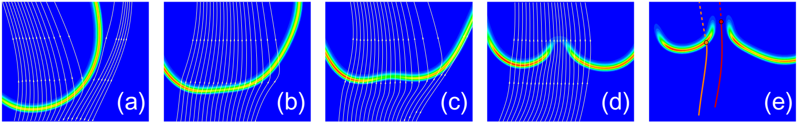




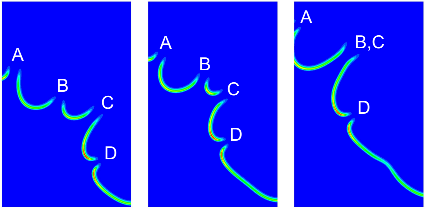
- Figure is "underside" (from fuel side of flame)
- Flame surface (isotherm) colored by local fuel consumption
- Cellular structures convex to fuel, robust extinction ridges

Localized hydrogen flame “extinction”

Analysis from 2D study

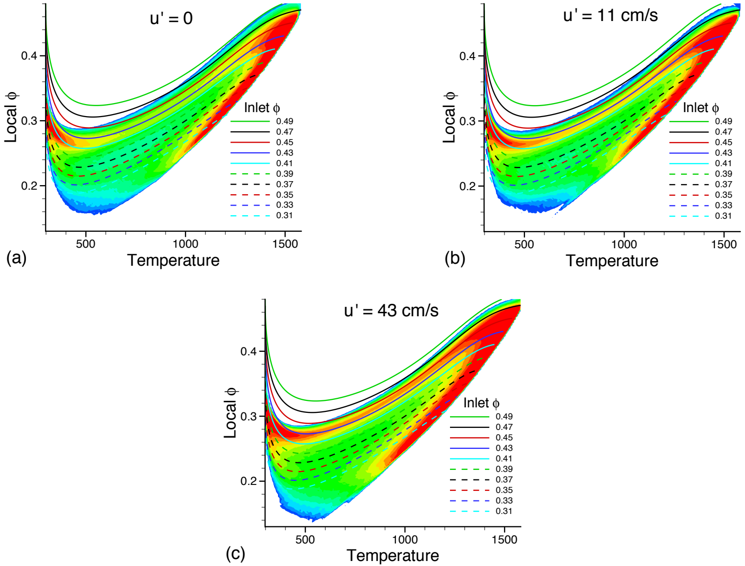


- Low-level localized strain event leads to onset of extinction.
- Lagrangian pathline analysis shows highly mobile fuel atoms diffuse “off-pathline”, no fuel leakage.

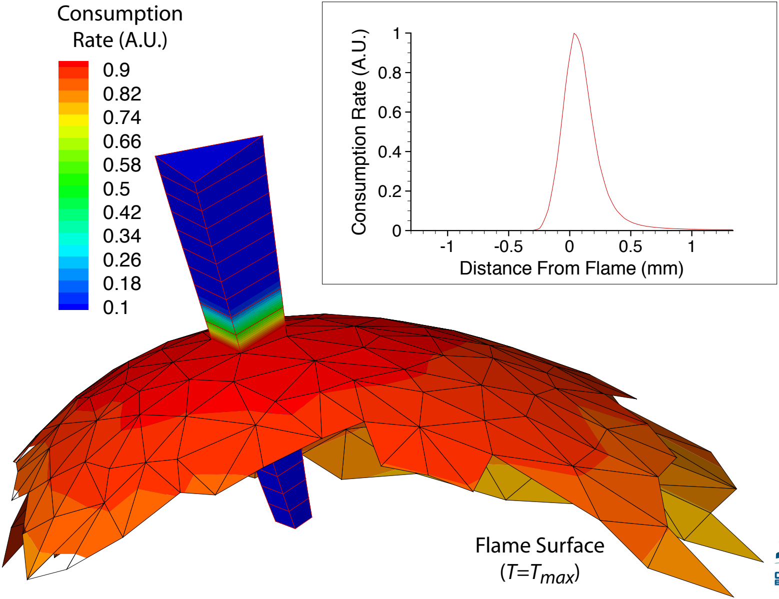


Extinction pockets once formed are very robust

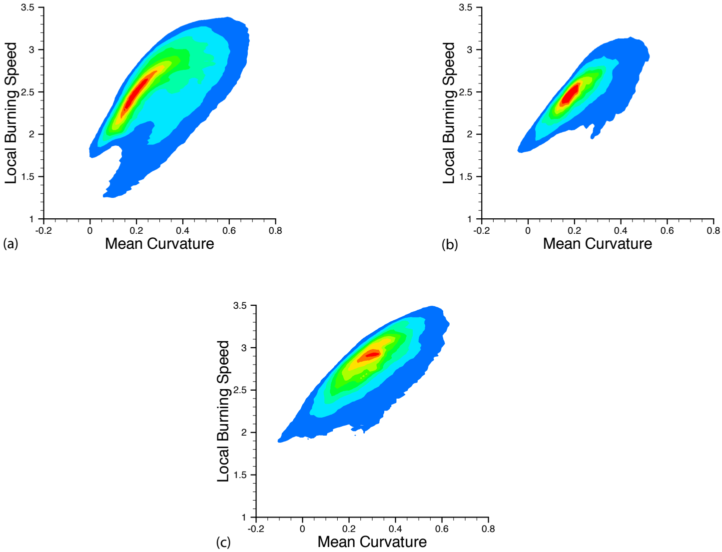
Local flame enrichment



Local consumption speed



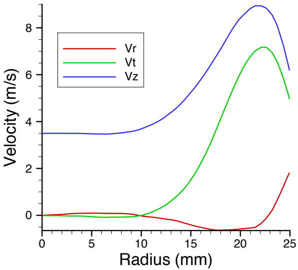
Flame speed versus curvature



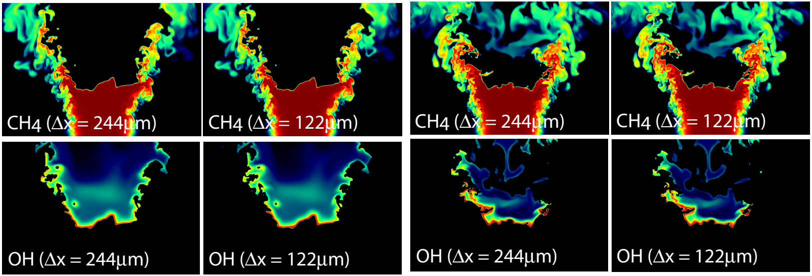
Low swirl burner simulations

Strategy:

- Treat outflow from the nozzle as an inflow boundary condition
  - Mean flow and turbulent intensities from measured data
  - Impose synthetic turbulence as a perturbation to mean inflow
- Simulate flow in a rectilinear domain sitting above the outflow
- Four cases
  - Hydrogen ($\phi = 0.37$) and methane ($\phi = 0.7$)
  - Laminar flame speed approximately 15 cm / sec
  - Two levels of mean flow and turbulence



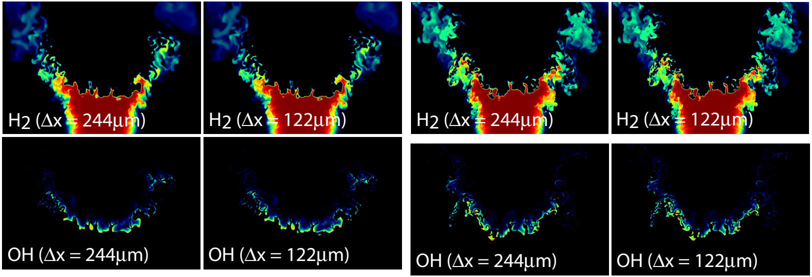
Methane swirl simulations



Weak Turbulence

Strong Turbulence

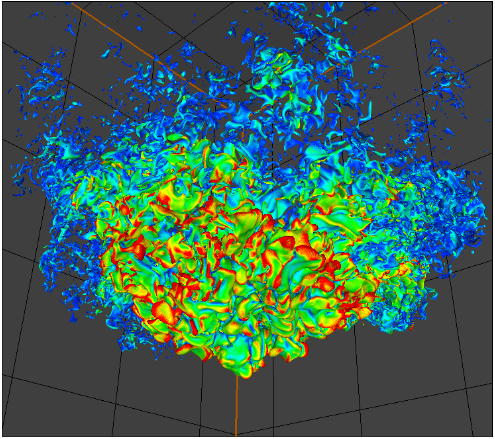
Hydrogen swirl simulations



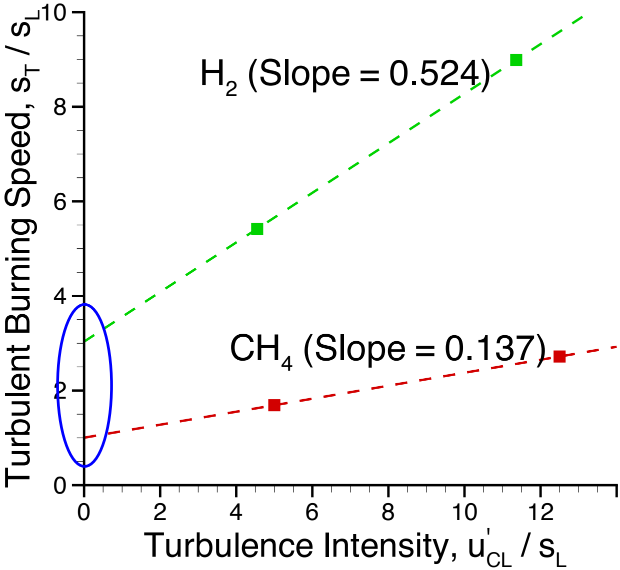
Weak Turbulence

Strong Turbulence

Hydrogen flame surface



Flame Speeds



Summary

Developed new methodology to simulate realistic turbulent flames based on exploiting mathematical structure of combustion problems

- Range of scales relevant to laboratory experiments
- Detailed chemistry and transport
- No explicit models for turbulence or turbulence / chemistry interaction
- Methodology being applied to hydrogen flames in low-swirl burner

Future work

- Closed chamber simulations
- Include nitrogen chemistry for emissions
- High-pressure simulations